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International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

Interfacial energy effects within the framework of strain gradient plasticity

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ARTICLE INFO

Article history:

Received 15 October 2008

Received in revised form 15 December 2008

Available online 25 December 2008

Keywords:

Gradient plasticity

Nonlocal continuum thermodynamics

Interfaces

Surface tension

Surface energy

ABSTRACT

In the framework of strain gradient plasticity, a solid body with boundary surface playing the role of a dissipative boundary layer endowed with surface tension and surface energy, is addressed. Using the so-called residual-based gradient plasticity theory, the state equations and the higher order boundary conditions are derived quite naturally for both the bulk material and the boundary layer. A phenomenological constitutive model is envisioned, in which the bulk material and the boundary layer obey (rate independent associative) *coupled* plasticity evolution laws, with kinematic hardening laws of differential nature for the bulk material, but of nondifferential nature for the layer. A combined global maximum dissipation principle is shown to hold. The higher order boundary conditions are discussed in details and categorized in relation to some peculiar features of the boundary surface, and their basic role in the coupling of the bulk/layer plasticity evolution laws is pointed out. The case of an internal interface is also studied. An illustrative example relating to a shear model exhibiting energetic size effects is presented. The theory provides a unified view on gradient plasticity with interfacial energy effects.

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1. Introduction

The term “interfacial energy effects” is often used in the literature related to strain gradient plasticity to denote phenomena that occur in a solid whose boundary surface is endowed with a surface tension and a surface energy, hence plays the role of a boundary layer interacting with the bulk material. The importance of these interfacial energy effects in determining the plastic constitutive behavior of micro- and nano-scale materials (for example, very thin films, wires and composites) has been abundantly proved in the literature, see e.g. Gudmundson (2004), Fredriksson and Gudmundson (2005, 2007a,b), Aifantis and Willis (2005, 2006), Aifantis et al. (2006), Borg and Fleck (2007), Abu Al-Rub et al. (2007), Abu Al-Rub (2008), Fleck and Willis (2008), and the references therein. A common view emerges from this literature, according to which, at micro/nano scales, the boundary surface (as e.g. grain boundary) plays the role of a boundary layer endowed with its own stored energy and obeys its own plasticity-like flow laws, which interferes with the plastic deformation mechanism of the adjacent bulk material. This layer's role is exercised at the microstructural level at which the layer contrasts, in more or less pronounced degree, the free motion of dislocations produced in the plastically deforming bulk material, with consequent dislocation pileups and formation of geometrically necessary dislocations (GNDs) (Ashby, 1970), such as to produce modifications, or even the arrest, of the plastic deformation mechanisms in the adjacent bulk mate-

rial. In other words, the boundary layer opposes itself to the action of the plastically deforming bulk material with a specific stiffness, which can be more or less pronounced according to the value of the surface tension and of the stored surface energy. At the extremes, when the surface tension and the surface energy are either infinite, or vanishing, correspondingly the layer proves to be either infinitely stiff, or infinitely soft. In the former case, the boundary layer constitutes a plastically rigid substrate at which the moving dislocations are blocked and the onset of plastic strain, ε^p , is fully impeded, i.e. $\varepsilon^p = \mathbf{0}$, whereas the applied action, say \mathbf{q} , can vary freely; in the second case, the boundary layer just disappears, then no obstacles are offered to the motion of dislocations, which thus can proceed outwards under null action, i.e. $\mathbf{q} = \mathbf{0}$, whereas plastic strain can vary freely. After Gurtin (2004), Gurtin and Anand (2005), Gurtin and Needleman (2005), the boundary surface is called *hard* (or *micro-hard*) in the first case, *free* (or *micro-free*) in the second case.

It also emerges from the afore-mentioned literature that strain gradient plasticity offers valid means to take into account interface energy effects. For this purpose, Gudmundson (2004), Fredriksson and Gudmundson (2005, 2007a,b) introduced a surface energy density, say $\varphi(\varepsilon^p)$, and used a virtual work principle to derive a higher order boundary condition in the form $\mathbf{q} = \partial\varphi/\partial\varepsilon^p$, which amounts to $\mathbf{q} = \mathbf{0}$ for a free boundary, and to $\varepsilon^p = \mathbf{0}$ for a hard boundary. Similar to the latter is the procedure by Abu Al-Rub et al. (2007), Abu Al-Rub (2008), as long with the one by Borg and Fleck (2007); the latter authors introduced two distinct surface energy potentials for the two faces of the internal interface (grain boundary). Aifantis and Willis (2005, 2006), Aifantis et al. (2006) also

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introduced a surface energy like the above, but derived the higher order boundary and interface conditions by means of a minimum principle of deformation-theory plasticity. Fleck and Willis (2008) considered a rigid-plastic interface with no hardening, at which plastic strain rate jumps are allowed to occur.

The main purpose of the present paper is to show that the residual-based strain gradient plasticity theory (Polizzotto and Borino, 1998; Polizzotto, 2003, 2007, 2008; Borino and Polizzotto, 2007) is able to account for interfacial energy effects in a quite natural way. For this purpose, it will suffice to consider a somewhat simplified gradient dependence. The above theory grounds upon the key concept of *insulation condition* (Polizzotto and Borino, 1998). This states that, for a nonsimple (either gradient-type, or integral-type) material, no long distance energy interchanges are allowed between the exterior world and the body, which thus constitutes a *constitutively closed system*. Obviously, if the body comprises a boundary surface and/or an interface with surface tension and surface energy stored therein, then the *closed system to consider must incorporate such boundary surface and interface*, otherwise the insulation condition fails to hold (Polizzotto, 2008).

It will be shown that the residual-based strain gradient plasticity theory is able to provide the pertinent restrictions on the constitutive equations for gradient plasticity both for the bulk material and the boundary layer(s). As customary within constitutive equation theory (Colemann and Gurtin, 1967; Germain et al., 1983; Lemaitre and Chaboche, 1990), this task is achieved entirely within nonlocal continuum thermodynamics by means of the (nonlocal) Clausius–Duhem inequality, but here the addition of some further restrictions is necessary (Polizzotto, 2007). These restrictions are: the *bilinear dissipation condition*, which amounts to assume that the Onsager reciprocity principle holds also in the present context, and that thus the dissipation power density exhibits a bilinear form in terms of independent plastic strain rate variables and related *affinities*; and the *locality recovery condition*, which requires that the residual be vanishing everywhere in the body undergoing a deformation mechanism with *uniform plastic strain*, so ensuring that the material behaves as a simple one correspondingly.

The theory in question, in the form in which it is formulated here and in previous papers, is able to describe strain localization (Polizzotto and Borino, 1998; Polizzotto, 2003) and size effects of energetic type (Polizzotto, 2003; Polizzotto, 2007; Borino and Polizzotto, 2007); its extension to dissipative size effects, or strengthening (Gurtin, 2004; Gurtin and Anand, 2005; Anand et al., 2005), is under study.

A research work similar to the present one was addressed by Polizzotto (2008), where an internal discontinuity interface was considered, but the surface energy was there assumed dependent only on a scalar measure of plastic strain and the boundary surface was treated as a standard one. This made it impossible to study all the interface energy effects and in particular the higher order boundary conditions in the intermediate situations in which the boundary surface is microscopically compliant. Indeed, the latter paper was written with the purpose to make a comparison between the present theory and the analogous one based on the virtual work principle (Fleck and Hutchinson, 2001; Gurtin, 2004; Gurtin and Anand, 2005; Gurtin and Needleman, 2005; Gudmundson, 2004; Fredriksson and Gudmundson, 2005; Abu Al-Rub et al., 2007). The latter comparison completes a previous one by Borino and Polizzotto (2007).

The paper is organized as follows. In Section 2 gradient plasticity with surface tension and surface energy allotted in the boundary surface is addressed. A thermodynamic procedure is applied to derive the state equations together with the expressions of the plastic dissipation power density and of the energy residual for both the bulk material and the boundary layer (Section 2.1). The

evolution laws for the coupled kinematically hardening bulk/layer system are given, which are shown to obey a combined global maximum dissipation principle. The problem of determining the stress and plastic strain state in a body being in a given total strain state and subjected to an assigned plastic strain rate field is shown to be governed by a minimum principle, which is equivalent to a PDE system (Section 2.2). The higher order boundary conditions are then discussed and categorized (Section 2.3). In Section 3, the existence of an internal interface is also discussed and the results of the previous section are consequently extended. In Section 4 an example is presented and discussed. Conclusions are in Section 5.

1.1. Notation

A compact notation is used, with boldface letters denoting vectors or tensors of any order. The scalar product between vectors or tensors is denoted with as many dots as the number of contracted index pairs. For instance, denoting by $\mathbf{u} = \{u_i\}$, $\mathbf{v} = \{v_i\}$, $\boldsymbol{\varepsilon} = \{\varepsilon_{ij}\}$, $\boldsymbol{\sigma} = \{\sigma_{ij}\}$, $\boldsymbol{\tau} = \{\tau_{ijk}\}$ and $\mathbf{A} = \{A_{ijkl}\}$ some vectors and tensors, one can write: $\mathbf{u} \cdot \mathbf{v} = u_i v_i$, $\boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \sigma_{ij} \varepsilon_{ji}$, $\mathbf{A} : \boldsymbol{\varepsilon} = \{A_{ijkl} \varepsilon_{hk}\}$, $\mathbf{A} : \boldsymbol{\tau} = \{A_{ijkl} \tau_{hjk}\}$. The summation rule for repeated indices holds and the subscripts denote components with respect to an orthogonal Cartesian co-ordinate system, say $\mathbf{x} = (x_1, x_2, x_3)$. An upper dot over a symbol denotes its time derivative, $\dot{\mathbf{u}} = \partial \mathbf{u} / \partial t$. The symbol ∇ denotes the spatial gradient operator, i.e. $\nabla \mathbf{u} = \{\partial_i u_j\}$. The symbol $:=$ means equality by definition. Other symbols will be defined in the text at their first appearance.

2. Gradient plasticity with boundary layer

For simplicity of exposition, in this section, a body of (open) domain V and boundary surface $S := \partial V$ is considered, in which S is featured by a surface tension and a surface energy. Interfaces with analogous features will be considered in next section.

2.1. Thermodynamic procedure

The considered body, referred to Cartesian orthogonal co-ordinates, say $\mathbf{x} = (x_1, x_2, x_3)$, undergoes small deformations. It comprises a continuous material occupying V and a boundary layer occupying S . The bulk material and the layer are endowed with free energies as

$$\psi = \psi_e(\boldsymbol{\varepsilon}^e) + \psi_p(\boldsymbol{\varepsilon}^p, \nabla \boldsymbol{\varepsilon}^p) \quad \text{in } V, \quad (1)$$

$$\psi^S = \psi^S(\boldsymbol{\varepsilon}^{pS}) \quad \text{on } S, \quad (2)$$

where $\boldsymbol{\varepsilon}^e$ and $\boldsymbol{\varepsilon}^p$ are elastic and plastic strains in V , such as $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$ gives the total strain, whereas $\nabla \boldsymbol{\varepsilon}^p$ denotes the spatial gradient of plastic strain; $\boldsymbol{\varepsilon}^{pS}$ denotes the plastic strain in the layer. Note that $\boldsymbol{\varepsilon}^p$ is assumed C^1 -continuous in $V \cup S$. This means that

$$\boldsymbol{\varepsilon}^{pS} = \boldsymbol{\varepsilon}^p \quad \text{on } S, \quad (3)$$

that is, *the layer deforms plastically as the adjacent bulk material*. As shown by (1), $\boldsymbol{\varepsilon}^p$ and $\nabla \boldsymbol{\varepsilon}^p$ play the role of internal variables. In the literature, other variables of this type are also considered in order to describe particular material behaviors, as for instance the Burgers tensor $\text{curl } \boldsymbol{\varepsilon}^p$ (Gurtin and Anand, 2005), the tensor $\text{curl } \mathbf{H}^p$, where \mathbf{H}^p is the plastic distortion, i.e. the plastic part of the displacement gradient (Gurtin, 2004), the plastic spin \mathbf{w}^p , i.e. the skew symmetric part of \mathbf{H}^p (Bardella, 2008), the accumulated plastic strain κ and its gradient (Abu Al-Rub, 2008; Polizzotto, 2007); but for simplicity here we disregard such additional internal variables (the extension of the obtained results such as to include the disregarded variables would be straightforward). The dependence of ψ^S on $\boldsymbol{\varepsilon}^{pS}$ indicates the capacity of the boundary layer to strain harden, with

consequent storage of free energy, the larger the more pronounced is its plastic deformation state.

2.1.1. Remark

A remark is here appropriate in regard to the relationship between the bulk and surface energies. Obviously, we can write $\psi^S = \ell^S \psi_0$, where ψ_0 is a bulk energy like ψ and ℓ^S is an internal length that represents the thickness of the layer, but this does not explain whether the plastic strain gradient has to be an argument of ψ^S , or not. We attempt to explain (at least in part) this point by considering S as an interface. Using the symbol \mathbf{e}^p instead of \mathbf{e}^{ps} for simplicity, we can write $\nabla \mathbf{e}^p = \nabla^{(s)} \mathbf{e}^p + \mathbf{n} \partial_n \mathbf{e}^p$, where \mathbf{n} is the outward unit normal vector to S , $\partial_n = \mathbf{n} \cdot \nabla$ is the normal derivative operator and $\nabla^{(s)} := \nabla - \mathbf{n} \partial_n$ is the surface gradient operator. Furthermore, let us assume that ψ^S also depends on $\nabla \mathbf{e}^p$. Denoting by h the small (but finite) thickness of the interface, we can write

$$\partial_n \mathbf{e}^p = \lim_{h \rightarrow 0} \frac{1}{h} \mathbf{n} \cdot [[\mathbf{e}^p]] \quad (4)$$

where $[[a]]$ denotes the jump of a across the interface. If \mathbf{e}^p is continuous across S , then $\partial_n \mathbf{e}^p$ exists finite, hence ψ^S may depend on it, but this is to be excluded if $\lim_{h \rightarrow 0} [[\mathbf{e}^p]]$ for $h \rightarrow 0$ is different from zero. In the latter case, in fact, $\partial_n \mathbf{e}^p$ is unbounded and thus ψ^S cannot depend on it. So, in general ψ^S may depend on $\nabla^{(s)} \mathbf{e}^p$, besides \mathbf{e}^p . Such dependence was formally studied in Polizzotto (2008), but its implications for the physics of the interface are still open to investigation. Here we simply assume that ψ^S depends only on the plastic strain tensor, as stated by (2).

In a generic elastic–plastic deformation mechanism of the entire system, starting from a given stress ($\boldsymbol{\sigma}$) and strain state, and characterized by strain rates $\dot{\mathbf{e}} = \dot{\mathbf{e}}^e + \dot{\mathbf{e}}^p$, due to the nonlocal nature of the material, some long distance energy interchanges occur within V and between V and S . We call *energy residual* (or simply *residual*) the power density transmitted to the generic particle from the rest of the body; more precisely, we denote P (power per unit volume) the residual at points of V , P^S (power per unit area) the residual at points of S . With this notion in mind (see e.g. Polizzotto and Borino (1998), Polizzotto (2003, 2007) for more information about it), and in consideration that the displacement field is continuous in $V \cup S$, the Clausius–Duhem inequality can be cast as follows:

$$D := \boldsymbol{\sigma} : \dot{\mathbf{e}} - \dot{\psi} + P \geq 0 \quad \text{in } V, \quad (5)$$

$$D^S := -\dot{\psi}^S + P^S \geq 0 \quad \text{on } S, \quad (6)$$

where D and D^S denote plastic dissipation power densities in the bulk material and in the boundary layer, respectively.

In relation to (6) it has to be noted that in the most part of the literature related to interfacial energy effects quoted at the beginning, it is assumed that the boundary layer is not dissipative, i.e. $D^S \equiv 0$. If one accepts this view, (6) should be replaced with the equality

$$-\dot{\psi}^S + P^S = 0 \quad \text{on } S, \quad (7)$$

meaning that the layer is a (reversible) system in which the energy residual P^S (surface power density transmitted to S by the bulk material) is entirely stored in S as surface free energy. However, in perfect similarity to the relation $\psi^S = \ell^S \psi_0$ used within the Remark above, we can also write $D^S = \ell^S D_0$ (where D_0 is some bulk dissipation density), so postulating a nonvanishing D^S . The introduction of a dissipative boundary surface makes it possible to further enforce the behavioral similarity between the layer and the bulk material. So, (6) will be used in the following. In the framework of gradient plasticity, dissipative boundary surfaces were introduced by Svedberg and Runesson (1998), Menzel and Steinmann (2000), Anand et al. (2005), Gurtin and Needleman (2005).

On expanding the time derivative of ψ and with the positions

$$\mathbf{X}^{(0)} := \frac{\partial \psi_p}{\partial \mathbf{e}^p}, \quad \mathbf{X}^{(1)} := \frac{\partial \psi_p}{\partial (\nabla \mathbf{e}^p)} \quad \text{in } V, \quad (8)$$

$$\mathbf{X} := \mathbf{X}^{(0)} - \nabla \cdot \mathbf{X}^{(1)} \quad \text{in } V, \quad (9)$$

inequality (5) can be recast in the form

$$D = \left(\boldsymbol{\sigma} - \frac{\partial \psi_e}{\partial \mathbf{e}^e} \right) : \dot{\mathbf{e}}^e + (\boldsymbol{\sigma} - \mathbf{X}) : \dot{\mathbf{e}}^p - \nabla \cdot (\mathbf{X}^{(1)} : \dot{\mathbf{e}}^p) + P \geq 0 \quad \text{in } V. \quad (10)$$

The second order tensor $\mathbf{X}^{(0)} = \{X_{ij}^{(0)}\}$ and the third order tensor $\mathbf{X}^{(1)} = \{X_{kij}^{(1)}\}$ in (8) are thermodynamic forces having the role of *hardening forces*, whereas the second order tensor $\mathbf{X} = \{X_{ij}\} = \{X_{ij}^{(0)} - X_{kij,k}^{(1)}\}$ denotes the *total back stress*; all these tensors are symmetric in the (i,j) indices. Since inequality (10) holds for whatever elastic–plastic deformation mechanism, including purely elastic ones (for which it is $\dot{\mathbf{e}}^p \equiv \mathbf{0}$ and $P \equiv 0$), it implies

$$\boldsymbol{\sigma} = \frac{\partial \psi^e}{\partial \mathbf{e}^e} \quad \text{in } V, \quad (11)$$

which is the elasticity stress–strain relation. Hence, assuming that (11) holds also in the case of elastic–plastic deformation mechanisms, inequality (10) reduces to

$$D = (\boldsymbol{\sigma} - \mathbf{X}) : \dot{\mathbf{e}}^p - \nabla \cdot (\mathbf{X}^{(1)} : \dot{\mathbf{e}}^p) + P \geq 0 \quad \text{in } V. \quad (12)$$

As explained in Section 1, the *bilinear dissipation condition* amounts to assuming that the dissipation power D is expected to exhibit a bilinear form in terms of independent plastic strain modes and related thermodynamic forces, or *affinities*, that is, in the present case, a form as

$$D = \hat{\boldsymbol{\sigma}} : \dot{\mathbf{e}}^p \quad \text{in } V, \quad (13)$$

where $\hat{\boldsymbol{\sigma}} = \{\hat{\sigma}_{ij}\}$ is some symmetric stress. Then, substituting from (13) into (10), one obtains

$$P = (\hat{\boldsymbol{\sigma}} - \boldsymbol{\sigma} + \mathbf{X}) : \dot{\mathbf{e}}^p + \nabla \cdot (\mathbf{X}^{(1)} : \dot{\mathbf{e}}^p). \quad (14)$$

The total bulk residual, applying the divergence theorem, proves to be

$$\int_V P dV = \int_V (\hat{\boldsymbol{\sigma}} - \boldsymbol{\sigma} + \mathbf{X}) : \dot{\mathbf{e}}^p dV + \int_S \mathbf{n} \cdot \mathbf{X}^{(1)} : \dot{\mathbf{e}}^p dS. \quad (15)$$

Next, following a procedure as for the bulk material and with the position

$$\mathbf{Q} := \frac{\partial \psi^S}{\partial \mathbf{e}^{ps}} \quad \text{on } S, \quad (16)$$

we can write, in similarity to (10) and (13),

$$D^S = -\mathbf{Q} : \dot{\mathbf{e}}^{ps} + P^S = \hat{\mathbf{q}} : \dot{\mathbf{e}}^{ps} \geq 0 \quad \text{on } S, \quad (17)$$

where $\hat{\mathbf{q}} = \{\hat{q}_{ij}\}$ denotes a (symmetric) higher order traction analogous to $\hat{\boldsymbol{\sigma}}$. From (17) we then obtain

$$P^S = (\mathbf{Q} + \hat{\mathbf{q}}) : \dot{\mathbf{e}}^{ps} \quad \text{on } S \quad (18)$$

and thus, with an integration over S ,

$$\int_S P^S dS = \int_S (\mathbf{Q} + \hat{\mathbf{q}}) : \dot{\mathbf{e}}^{ps} dS. \quad (19)$$

The *insulation condition* requires that the total amount of the energy residual of the closed system be identically vanishing, i.e.

$$\int_V P dV + \int_S P^S dS = 0, \quad (20)$$

for whatever elastic–plastic deformation mechanism. Eq. (20), substituting from (15) and (19), and accounting for the bulk/layer continuity of plastic strain, Eq. (3), gives

$$\int_V (\hat{\sigma} - \sigma + \mathbf{X}) : \dot{\varepsilon}^p dV + \int_S (-\mathbf{q} + \mathbf{Q} + \hat{\mathbf{q}}) : \dot{\varepsilon}^p dS = 0, \quad (21)$$

where we have posed

$$\hat{\mathbf{q}} := -\mathbf{n} \cdot \mathbf{X}^{(1)} \quad \text{on } S. \quad (22)$$

Eq. (21) implies the following equations:

$$\hat{\sigma} = \sigma - \mathbf{X} \quad \text{in } V, \quad (23)$$

$$\hat{\mathbf{q}} = \mathbf{q} - \mathbf{Q} \quad \text{on } S. \quad (24)$$

Eqs. (23) and (24) identify $\hat{\sigma}$ and $\hat{\mathbf{q}}$ as *relative stresses*. Recognizing that the quantity \mathbf{q} of (22) is the *applied tension*, that is, the higher order action of the bulk material upon the layer, substituting from (23) and (24) into (13), (14), (17) and (18) gives

$$D = (\sigma - \mathbf{X}) : \dot{\varepsilon}^p \geq 0, \quad P = \nabla \cdot (\mathbf{X}^{(1)} : \dot{\varepsilon}^p), \quad \text{in } V, \quad (25)$$

$$D^S = (\mathbf{q} - \mathbf{Q}) : \dot{\varepsilon}^p \geq 0, \quad P^S = \mathbf{q} : \dot{\varepsilon}^p, \quad \text{on } S, \quad (26)$$

which are the pertinent expressions of the dissipation power density and of the energy residual in the bulk and in the layer.

The *locality recovery condition* requires that the residual vanishes everywhere in the closed system for whatever *uniform* plastic strain rate mechanism. This serves to guarantee that the gradient material behaves as a simple material in the absence of nonlocality sources. It imposes restrictions on the free energy function, whereby the latter function, in the limit conditions of uniform plastic strain, must tend to behave as being dependent on $\nabla \varepsilon^p$ homogeneously with a degree larger than one (Polizzotto et al., 2006; Polizzotto, 2007). If this requisite is satisfied, as we assume, the higher order hardening force $\mathbf{X}^{(1)}$ (which correspondingly tends to depend on $\nabla \varepsilon^p$ homogeneously with a degree larger than zero) will vanish whenever ε^p is uniformly distributed.

At the end of the above procedure, we have derived the state equations for the bulk material, i.e. Eqs. (8), (9) and (11), together with the related expressions of the plastic dissipation and of the residual in Eq. (25), and analogously for the layer, Eqs. (16) and (26). Eq. (9) is a PDE system describing the bulk hardening law, which relates the total back stress, \mathbf{X} , to the plastic strain, ε^p . This PDE system can, at least in principle, be solved to express the ε^p field in terms of the \mathbf{X} field, provided that the appropriate (higher order) boundary conditions are taken into consideration. These boundary conditions are dictated by some bulk/layer compatibility conditions, as explained next.

2.2. Evolution laws

On the basis of the plastic dissipation power density expressions in (25) and (26), which represent thermodynamic restrictions upon the constitutive equations, the evolution laws for the bulk material and for the layer, in the hypothesis of rate independent associative plasticity, can be cast, using a standard notation, as follows:

$$f := \phi(\sigma - \mathbf{X}) - \sigma_y \leq 0, \quad \dot{\lambda} \geq 0, \quad \dot{\lambda}f = 0, \quad \text{in } V, \quad (27)$$

$$\dot{\varepsilon}^p = \dot{\lambda} \phi_{,\sigma} \quad \text{in } V, \quad (28)$$

$$f^S := \phi^S(\mathbf{q} - \mathbf{Q}) - \sigma_y^S \leq 0, \quad \dot{\lambda}^S \geq 0, \quad \dot{\lambda}^S f^S = 0, \quad \text{on } S, \quad (29)$$

$$\dot{\varepsilon}^p = \dot{\varepsilon}^{pS} = \dot{\lambda}^S \phi_{,\mathbf{q}}^S \quad \text{on } S. \quad (30)$$

Here, the (convex smooth) functions ϕ and ϕ^S are degree-one positively homogeneous, and the notation $\phi_{,\alpha} = \partial \phi / \partial \alpha$ is used. Also, σ_y is the yield strength of the bulk material, whereas σ_y^S denotes the surface tension, a characteristics of the boundary layer with the role

of surface yield strength; $\dot{\lambda}$ and $\dot{\lambda}^S$ are the conventional plastic activation coefficients in the bulk and the layer. It can be easily proved that the dissipation nonnegativity requirements in (25) and (26) are fulfilled for whatever set of variables complying with (27)–(30).

Eqs. (27)–(30) describe the constitutive behavior of a coupled kinematically hardening bulk/layer system, in which \mathbf{X} and \mathbf{Q} play the role of bulk and layer backstresses, respectively. Considering the higher order traction scaled by $1/\ell^S$, so obtaining $\mathbf{q} \rightarrow \mathbf{q}/\ell^S$, let the (\mathbf{q}/ℓ^S) -space be imbedded into the σ -space. Then, the yield surfaces $f = 0$ and $f^S = 0$ (the former being related to points adjacent to S) exhibit, for $\dot{\varepsilon}^p \neq \mathbf{0}$, parallel tangent planes at the respective activation stress points, Fig. 1.

The combined plasticity flow laws (27)–(30) admit a global *maximum dissipation principle*. This can be cast in the form:

$$\left. \begin{aligned} \max_{\hat{\sigma}, \hat{\mathbf{q}}} \int_V \hat{\sigma} : \dot{\varepsilon}^p dV + \int_S \hat{\mathbf{q}} : \dot{\varepsilon}^p dS \\ \text{s.t. } \phi(\hat{\sigma}) - \sigma_y \leq 0 \text{ in } V, \quad \phi^S(\hat{\mathbf{q}}) - \sigma_y^S \leq 0 \text{ on } S \end{aligned} \right\} \quad (31)$$

where “s.t.” means “subject to” and $\dot{\varepsilon}^p$ is a C^1 -continuous field assigned in $V \cup S$. It is an easy task to show that the Euler–Lagrange equations associated to (31) coincide with (27)–(30), but this point is skipped for brevity.

In analogy to classical plasticity theory, we can state that the optimal objective value of problem (31), say \mathcal{D} , is a functional of the form

$$\mathcal{D}[\dot{\varepsilon}^p] = \int_V D(\dot{\varepsilon}^p) dV + \int_S D^S(\dot{\varepsilon}^p) dS. \quad (32)$$

Here, $D(\dot{\varepsilon}^p)$ and $D^S(\dot{\varepsilon}^p)$ are the bulk and surface dissipation functions, both degree-one positively homogeneous, and satisfy the equalities

$$\hat{\sigma} = \sigma^*(\dot{\varepsilon}^p) := \frac{\partial D}{\partial \dot{\varepsilon}^p}, \quad \hat{\mathbf{q}} = \mathbf{q}^*(\dot{\varepsilon}^p) := \frac{\partial D^S}{\partial \dot{\varepsilon}^p} \Big|_{\dot{\varepsilon}^p = \dot{\varepsilon}^p}, \quad (33)$$

where $\sigma^*(\dot{\varepsilon}^p)$ and $\mathbf{q}^*(\dot{\varepsilon}^p)$ are the *dissipative stresses* corresponding to $\dot{\varepsilon}^p$. The latter equations hold for whatever nonzero $\dot{\varepsilon}^p$, but lose meaning for $\dot{\varepsilon}^p = \mathbf{0}$, in which case $f(\hat{\sigma}) < 0$ and $f^S(\hat{\mathbf{q}}) < 0$.

It is to be noted that, in spite of the bulk material being a non-simple material, the principle (31) is local in nature. It in fact just provides the relative stress state $\hat{\sigma}$ and $\hat{\mathbf{q}}$ in the system, under which the assigned plastic mechanism can actually occur. The non-simple nature of the material comes into play if, after having solved problem (31), one wishes to evaluate the corresponding stress (σ) and plastic strain (ε^p) states, *the total strain field ε being known*. For this purpose, using the relations 8, 11 and 23, we arrive at the PDE system:

$$\left. \begin{aligned} \mathbf{X}^{(0)}(\varepsilon^p, \nabla \varepsilon^p) - \nabla \cdot \mathbf{X}^{(1)}(\varepsilon^p, \nabla \varepsilon^p) - \sigma(\varepsilon - \varepsilon^p) &= -\sigma^*(\mathbf{x}) \quad \text{in } V \\ \mathbf{Q}(\varepsilon^p) + \mathbf{n} \cdot \mathbf{X}^{(1)}(\varepsilon^p, \nabla \varepsilon^p) &= -\mathbf{q}^*(\mathbf{x}) \quad \text{on } S \end{aligned} \right\} \quad (34)$$

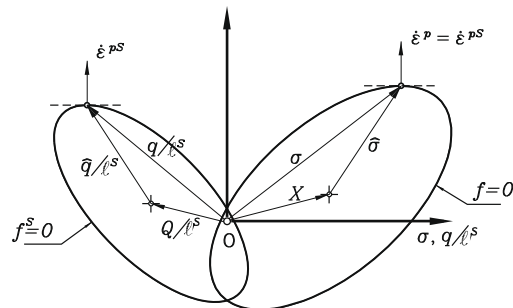


Fig. 1. Sketch showing the yield surfaces of the bulk material ($f = 0$) and of the boundary layer ($f^S = 0$) in the superposed σ -space and (\mathbf{q}/ℓ^S) -space. At yield, by the higher order boundary condition, it is $\dot{\varepsilon}^p = \dot{\varepsilon}^{pS}$, hence the tangent planes (dashed lines) are parallel.

where $\sigma^*(\mathbf{x})$ and $\mathbf{q}^*(\mathbf{x})$ are the stress fields derived as the solution to problem (31). At least in principle, the PDE system (34) can be solved to obtain the unknown \mathbf{e}^p field in $V \cup S$, which in turn can be used to compute σ and \mathbf{X} . Problem (34) admits a variational formulation which – under condition of convexity of ψ_e , ψ_p and ψ_p^S – consists in the minimization of the functional

$$Y[\mathbf{e}^p] : P = \int_V [\psi_e(\mathbf{e} - \mathbf{e}^p) + \psi_p(\mathbf{e}^p, \nabla \mathbf{e}^p) + \sigma^* : \mathbf{e}^p] dV + \int_S [\psi^S(\mathbf{e}^p) + \mathbf{q}^* : \mathbf{e}^p] dS \quad (35)$$

subject to the C^1 -continuity condition of \mathbf{e}^p on $V \cup S$. In fact, the first variation of (35), after application of the divergence theorem and using the notations (8), (11) and (16), reads:

$$\delta Y = \int_V (-\sigma + \mathbf{X}^{(0)} - \nabla \cdot \mathbf{X}^{(1)} + \sigma^*) : \delta \mathbf{e}^p dV + \int_S (\mathbf{n} \cdot \mathbf{X}^{(1)} + \mathbf{Q} + \mathbf{q}^*) : \delta \mathbf{e}^p dS \quad (36)$$

and thus the stationarity conditions of (35) coincide with the equations in (34). Since, by the convexity of ψ_e , ψ_p and ψ^S , it is $\delta^2 Y > 0$ for whatever nontrivial $\delta \mathbf{e}^p$ field, follows that the stationarity solution to (35) minimizes Y , and conversely.

2.3. The higher order boundary conditions

If the interfacial effects are disregarded (this almost always is the case in the previous formulations of the residual-based gradient plasticity theory), we have to set $\psi^S = \sigma_y^S = D^S = 0$, hence $\mathbf{Q} = \mathbf{q}^* = \mathbf{0}$, such that the surface integral on the r.h. side of (21) reduces to $-\int_S \mathbf{q} : \dot{\mathbf{e}}^p dS$, and as a consequence Eq. (21) gives directly the well-known higher order boundary conditions (Gurtin, 2004; Gurtin and Anand, 2005; Gurtin and Needleman, 2005; Polizzotto, 2007), that is:

$$\dot{\mathbf{e}}^p = \mathbf{0}, \quad \text{but } \mathbf{q} \text{ free, on } S_c^{(1)}, \quad (37)$$

$$\mathbf{q} = \mathbf{0}, \quad \text{but } \dot{\mathbf{e}}^p \text{ free, on } S_f^{(1)}. \quad (38)$$

where $S_c^{(1)}$ is the *hard* portion of S , $S_f^{(1)}$ the *free* one, and $S = S_c^{(1)} \cup S_f^{(1)}$. As pointed out by Polizzotto (2007), the above boundary conditions hold both in time-finite and rate forms due to the fact that S is fixed (which is in contrast to the moving elastic/plastic internal boundary, where the higher order boundary conditions must be written in rate form and read $\dot{\mathbf{e}}^p = \dot{\mathbf{q}} = \mathbf{0}$). Of course, correspondingly, Eqs. (24), (26), (6) and (7) lose meaning and do not hold any longer.

We thus have that, in the absence of interfacial energy effects, the thermodynamic procedure of Section 2.1 leads straightforwardly to the pertinent higher order boundary conditions (37) and (38). Instead, things are a littlebit more complex in the presence of interfacial energy effects, since then (37) and (38) do not hold and the actual higher order boundary conditions are expressed by the strain rate equality (30), which couples together the plasticity flow laws of the bulk material and the boundary layer.

In order to better specify the latter boundary conditions, let us first observe that a boundary layer with infinite surface energy, but finite surface tension, proves to be *plastically rigid* just like in the opposite case, i.e. infinite surface tension, but finite surface energy. This implies that the layer model in consideration can be thought of to be characterized by a surface tension, σ_y^S , that can be made to vary from zero to infinite, and by a *bounded* surface energy ($0 \leq \psi^S < \infty$).

Additionally, let us note that (29) and (30) dictate a continuity condition of the plastic strain rate at all contact points between the bulk material and the surface layer. This condition, implemented by (30), can be interpreted as a (higher order) boundary

constraint imposed to the bulk material, under which the bulk plastic strain at points adjacent to the layer takes on values prescribed by the *plastically stiff* layer. Therefore, (30) rewritten in time-integrated form, i.e.

$$\mathbf{e}^p = \mathbf{e}^{pS} = \int_0^t \dot{\lambda}^S(\tau) \phi_{\mathbf{q}}^S(\tau) d\tau \quad \text{on } S, \quad (39)$$

constitutes the higher order boundary condition to be associated with the PDE system (8) and (9). For $\sigma_y^S \rightarrow \infty$, obviously it is $\dot{\lambda}^S = 0$ at all times, hence $\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{pS} = \mathbf{0}$, that is, the layer is plastically rigid, thus the case of hard boundary surface previously considered is obtained correspondingly as a special case of (39).

Let us further note that, for $\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{pS} \neq \mathbf{0}$, the applied tension \mathbf{q} finds itself on the yield surface, $\phi^S(\mathbf{q} - \mathbf{Q}) = \sigma_y^S > 0$, and it is thus uniquely determinate in the form (see Fig. 1):

$$\mathbf{q} = \mathbf{Q}(\dot{\mathbf{e}}^p) + \hat{\mathbf{q}}(\dot{\mathbf{e}}^p) = \mathbf{Q}(\dot{\mathbf{e}}^p) + \mathbf{q}^*(\dot{\mathbf{e}}^p) \quad \text{on } S, \quad (40)$$

where $\hat{\mathbf{q}}(\dot{\mathbf{e}}^p) = \mathbf{q}^*(\dot{\mathbf{e}}^p)$ is the (nonvanishing) dissipative higher order traction relative to $\dot{\mathbf{e}}^p$, Eq. (33)₂. We may be tempted to choose as higher order boundary condition the stress equation (40) instead of the strain Eq. (39). But, since for $\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{pS} = \mathbf{0}$, and thus $\mathbf{q}^*(\dot{\mathbf{e}}^p)$ is indeterminate, Eq. (40) does not hold (it in general would be $\mathbf{q} \neq \mathbf{Q}$, but $\phi^S(\mathbf{q} - \mathbf{Q}) < \sigma_y^S$ correspondingly), whereas (39) is still fulfilled, it follows that such a choice would imply the nonattractive idea that, at every point, the higher order boundary conditions may change from a strain to a stress form and viceversa during the deformation process. Also because (40) contains the plastic strain rate, it can be concluded that – in the considered condition in which $\sigma_y^S > 0$ – Eq. (39) can be viewed as the appropriate higher order boundary condition.

However, (39) is meaningful only for $\sigma_y^S > 0$. In fact, if $\sigma_y^S = 0$, by (29)₁, it must necessarily be

$$\mathbf{q} = \mathbf{Q}(\dot{\mathbf{e}}^p) \quad \text{on } S. \quad (41)$$

Correspondingly, the layer becomes *nondissipative* ($D^S \equiv 0$), and loses its plastic stiffness ($\mathbf{q}^* = \mathbf{0} \forall \dot{\mathbf{e}}^p$), the yield surface $f^S = 0$ degenerates into a single point, which implies that the layer becomes *plastically soft*, meaning that the plastic strain rate $\dot{\mathbf{e}}^{pS}$ is *indeterminate*.

We thus can conclude that, in the latter case of plastically soft layer ($\sigma_y^S = 0$), the stress condition (41) is to be viewed as the appropriate higher order boundary condition, whereas correspondingly the layer's plastic strain rate, $\dot{\mathbf{e}}^{pS}$, takes on the values dictated by the adjacent bulk material. In particular, if in addition to $\sigma_y^S = 0$, it is $\mathbf{Q} \equiv \mathbf{0}$ (null surface energy), the higher order boundary condition (41) simplifies in $\mathbf{q} = \mathbf{0}$, which corresponds to the case of free boundary surface previously mentioned.

From the foregoing analysis it follows that the higher order boundary conditions for a boundary surface, using a terminology similar to one suggested by Gurtin (2004), Gurtin and Anand (2005), Gurtin and Needleman (2005), can be specified as in the following:

- (1) $\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{pS} = \mathbf{0}$, but \mathbf{q} free, for a *hard boundary surface*, i.e. one endowed with an infinite surface tension ($\sigma_y^S \rightarrow \infty$). Dislocations cannot penetrate the boundary with consequent pileups.
- (2) $\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{pS} \neq \mathbf{0}$, but \mathbf{q} not necessarily equal to $\mathbf{Q}(\dot{\mathbf{e}}^p)$, for a *stiff boundary surface*, i.e. a boundary surface with a nonzero (but finite) surface tension. The plastic mechanism is activated at a bulk/layer point when $f = f^S = 0$, which occurs after some time from the instant in which $f = 0$ at the involved bulk point. Dislocations are blocked at the boundary until the plastic mechanism is activated, then can traverse the boundary and move out, but a part of them may accumulate therein to promote the layer's hardening (if any).

- (3) $\mathbf{q} = \mathbf{Q}(\mathbf{e}^p)$, whereas the free $\dot{\mathbf{e}}^{ps}$ equals $\dot{\mathbf{e}}^p$, for a *soft boundary surface*, i.e. a boundary surface with null surface tension ($\sigma_y^s = 0$), but a nonzero surface energy. The plastic mechanism is activated at a bulk/layer point as soon as $f = 0$ at the bulk point. Dislocations behave as in the case of stiff layer, but with no blocking period.
- (4) $\mathbf{q} = \mathbf{0}$, but $\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{ps}$ free, for a *free boundary surface*, i.e. one with zero surface tension and zero surface energy. Dislocations can freely traverse the boundary and move out.

Note that case (1) (hard boundary surface) is a limit condition of case (2) (stiff boundary surface) for $\sigma_y^s \rightarrow \infty$, and that case (4) (free boundary surface) is a limit condition of case (3) (soft boundary surface) for $(\sigma_y^s, \psi^s) \rightarrow 0$.

On the basis of what precedes, in the general case in which the boundary surface is one with a surface tension and a surface energy, we can state that the higher order boundary conditions generate the coupling between the plasticity flow laws of the boundary layer and the analogous laws of the adjacent bulk material. More precisely, the boundary conditions consist either in the plastic strain continuity condition (39) for a *plastically stiff boundary surface* ($\sigma_y^s > 0$) – which becomes a plastic strain vanishing condition in the limit case of a hard boundary surface – or in the equality condition between the applied tension and the layer hardening force, Eq. (41), for a *plastically soft boundary surface*, ($\sigma_y^s = 0$) – which becomes an applied tension null condition in the limit case of a free boundary surface.

In concluding this section, let us remark that the results here derived are substantially coincident with results of the mentioned literature on interfacial energy effects. This is true in spite of the fact that in most part of this literature the surface energy is often taken in a form including a linear term, like $\psi^s = (1/2)\beta\|\mathbf{e}^p\|^2 + \gamma\|\mathbf{e}^p\|$, where β is the surface hardening modulus and γ the surface tension, see e.g. Aifantis et al. (2006), Abu Al-Rub (2008). A consequence of this writing is that the power density D^s is no longer dissipated as heat, but instead stored in the layer, which therefore proves to be nominally nondissipative. As previously noted, the formulation given here enhances the similarity between the layer and the bulk in their plastic constitutive behavior.

3. Gradient plasticity with boundary and interface layers

In this section, let us consider a body with the boundary surface S and an (internal) interface S^l endowed with surface tension and surface energy. For simplicity, S^l is assumed as the boundary surface of an inclusion of (open) domain V_2 , such that $V = V_1 \cup V_2$, but other geometries may also be considered (Polizzotto, 2008). In principle, we admit the existence of displacement jumps as $\mathbf{d} := \mathbf{u}_2 - \mathbf{u}_1$ (e.g. due to crack or sliding of the interface), as well as plastic strain jumps as $[[\mathbf{e}^p]] := \mathbf{e}_1^p - \mathbf{e}_2^p$ across S^l . The case in which such jumps are absent will be also investigated in the following. The unit normal vector to the (regular) interface S^l is taken oriented from V_1 to V_2 . We assume that the plastic strain in S^l , say \mathbf{e}^{pl} , is linearly distributed in the (infinitesimal) thickness and denote \mathbf{e}_m^{pl} its mean value. This simplified picture of the through-thickness plastic strain distribution enables us to assert the continuity of plastic strain at the two sides of S^l , i.e.

$$\mathbf{e}_\alpha^{pl} = \mathbf{e}_\alpha^p \quad \text{on } S_\alpha^l, \quad (\alpha = 1, 2), \quad (42)$$

in which S_α^l denotes the side of S^l adjacent to V_α . The (finite) surface energy of S^l is defined as

$$\psi^l = \psi^l(\mathbf{e}_m^{pl}) \quad \text{on } S^l, \quad (43)$$

where, by (42),

$$\mathbf{e}_m^{pl} = \frac{1}{2}(\mathbf{e}_1^p + \mathbf{e}_2^p) \quad \text{on } S^l. \quad (44)$$

The possible dependence of ψ^l on the jump $[[\mathbf{e}^p]]$ is here considered negligible. Fleck and Willis (2008) considered viscoplastic models with interfaces unable to store energy (i.e. $\psi^l \equiv 0$), but with evolution laws in terms of both $[[\mathbf{e}^p]]$ and \mathbf{e}_m^{pl} .

The Clausius–Duhem inequality for S^l takes on the form:

$$D^l := \mathbf{t}^l \cdot \dot{\mathbf{d}} - \dot{\psi}^l + P^l \geq 0 \quad \text{on } S^l, \quad (45)$$

where $\mathbf{t}^l := \mathbf{n} \cdot \boldsymbol{\sigma}|_{S^l}$ is the (continuous) traction across S^l , and P^l denotes the surface residual in S^l (long distance power per unit area transmitted to S^l from the rest of the body). Eqs. (1), (2), (5) and (6) hold also in the present section.

The previous procedure, from the beginning of Section (2.1) till Eq. (18), is still valid, except for Eq. (15), which has to be modified by adding to the r.h. side the integral term

$$I := \int_{S^l} [[\mathbf{n} \cdot \mathbf{X}^{(1)} : \dot{\mathbf{e}}^p]] dS = - \sum_{\alpha=1}^2 \int_{S^l} (-1)^\alpha \mathbf{n} \cdot \mathbf{X}_\alpha^{(1)} : \dot{\mathbf{e}}_\alpha^p dS. \quad (46)$$

This is the contribution from the interface and is here explicitly written for subsequent use. Applying the same procedure to the interface, by the bilinear dissipation condition we can write

$$D^l = \mathbf{t}^l \cdot \dot{\mathbf{d}} + \sum_{\alpha=1}^2 \hat{\mathbf{q}}_\alpha : \dot{\mathbf{e}}_\alpha^p, \quad (47)$$

where the quantities $\hat{\mathbf{q}}_\alpha$, ($\alpha = 1, 2$), are some (symmetric) higher order tractions (analogous to $\hat{\boldsymbol{\sigma}}$ and $\hat{\mathbf{q}}$ previously introduced). Comparing (47) with (45), expanding the time derivative of ψ^l and with the notation

$$\mathbf{Q}^l := \frac{\partial \psi^l}{\partial \mathbf{e}_m^p} \quad \text{on } S^l, \quad (48)$$

(referred to as the *interface hardening force*) we then have

$$P^l = \sum_{\alpha=1}^2 \left(\hat{\mathbf{q}}_\alpha + \frac{1}{2} \mathbf{Q}^l \right) : \dot{\mathbf{e}}_\alpha^p \quad \text{on } S^l, \quad (49)$$

then, with an integration upon S^l , we obtain

$$\int_{S^l} P^l dS = \sum_{\alpha=1}^2 \int_{S^l} \left(\hat{\mathbf{q}}_\alpha + \frac{1}{2} \mathbf{Q}^l \right) : \dot{\mathbf{e}}_\alpha^p dS. \quad (50)$$

The insulation condition now reads, instead of (20):

$$\int_V P dV + \int_S P^s dS + \int_{S^l} P^l dS = 0. \quad (51)$$

From this equation, remembering the missed term (46), we can obtain, besides to Eqs. (11), (12) and (21) with all the related consequences, i.e. Eqs. (23)–(26), also the following one:

$$\sum_{\alpha=1}^2 \int_{S^l} \left(-\mathbf{q}_\alpha + \hat{\mathbf{q}}_\alpha + \frac{1}{2} \mathbf{Q}^l \right) : \dot{\mathbf{e}}_\alpha^p dS = 0. \quad (52)$$

Here, in analogy to the previous section, we have introduced the higher order tractions \mathbf{q}_α , ($\alpha = 1, 2$), defined as

$$\mathbf{q}_\alpha := (-1)^\alpha \mathbf{n} \cdot \mathbf{X}_\alpha^{(1)} \quad (\alpha = 1, 2), \quad (53)$$

to denote the *applied tensions* upon the two sides of the interface by the adjacent bulk material, respectively.

The displacement jump \mathbf{d} is considered sometimes for grain boundary analyses, see e.g. Cermelli and Gurtin (2002), in which case the jump of plastic strain across the interface is likely nonvanishing. In this case the identity (52) yields

$$\hat{\mathbf{q}}_\alpha = \mathbf{q}_\alpha - \frac{1}{2} \mathbf{Q}^l, \quad (\alpha = 1, 2), \quad \text{on } S^l, \quad (54)$$

such that, by (47) and (49),

$$D^I = \mathbf{t}^I \cdot \dot{\mathbf{d}} + \sum_{\alpha=1}^2 \left(\mathbf{q}_\alpha - \frac{1}{2} \mathbf{Q}^I \right) : \dot{\mathbf{e}}_\alpha^p \geq 0 \quad \text{on } S^I, \quad (55)$$

$$P^I = \sum_{\alpha=1}^2 \mathbf{q}_\alpha : \dot{\mathbf{e}}_\alpha^p \quad \text{on } S^I. \quad (56)$$

Eq. (55), which holds also for $\dot{\mathbf{d}}$ being null identically, enables one to take into account the case in which the bulk material is still in an elastic state on one side, but plastically deforming on the other side (Fredriksson and Gudmundson, 2007a). However, a common view in the analyses of interface problems (like the grain boundary problems) is to consider null the plastic strain jump across S^I , i.e. $\mathbf{e}_1^p = \mathbf{e}_2^p$ (Aifantis and Willis, 2005, 2006; Aifantis et al., 2006; Borg and Fleck, 2007; Abu Al-Rub, 2008). In this case, (52) gives, besides to $\dot{\mathbf{e}}_m^{pl} = \dot{\mathbf{e}}^p$:

$$\sum_{\alpha=1}^2 \dot{\mathbf{q}}_\alpha = \langle \mathbf{q} \rangle - \mathbf{Q}^I \quad \text{on } S^I, \quad (57)$$

$$D^I = \langle \mathbf{q} \rangle - \mathbf{Q}^I : \dot{\mathbf{e}}^p \geq 0 \quad \text{on } S^I, \quad (58)$$

$$P^I = \langle \mathbf{q} \rangle : \dot{\mathbf{e}}^p \quad \text{on } S^I. \quad (59)$$

where we have posed

$$\langle \mathbf{q} \rangle := \mathbf{q}_1 + \mathbf{q}_2. \quad (60)$$

The latter equations hold together with (11) and (23)–(26).

As for the evolution laws, we can add to Eqs. (27)–(30) the equations relative to the interface. Limiting ourselves to the case of null plastic strain jump across S^I , on the basis of (58) we can analogously write

$$f^I = \phi^I(\langle \mathbf{q} \rangle - \mathbf{Q}^I) - \sigma_y^I \leq 0, \quad \lambda^I \geq 0, \quad \lambda^I f^I = 0 \quad \text{on } S^I, \quad (61)$$

$$\dot{\mathbf{e}}^p = \dot{\mathbf{e}}^{pl} = \lambda^I \phi_{,\langle \mathbf{q} \rangle}^I \quad \text{on } S^I, \quad (62)$$

where ϕ^I is a convex smooth degree-one positively homogeneous function, and σ_y^I is the surface tension of S^I . Interpretations and comments similar to the ones presented for Eqs. (27)–(30) can be repeated here. In particular, the coupling role of (62) is to be pointed out, meaning that the bulk plastic strain at points adjacent to S^I equals the interface plastic strain. Also, the interface S^I is dissipative as far as $\sigma_y^I > 0$, but is nondissipative if $\sigma_y^I = 0$. In the latter case, the interface becomes *plastically soft*, it deforms following the adjacent bulk material, whereas the related yield surface reduces to a single point and thus

$$\langle \mathbf{q} \rangle = \mathbf{Q}^I \quad \text{on } S^I. \quad (63)$$

This equality replaces (62) as higher order boundary condition in the case of vanishing surface tension ($\sigma_y^I = 0$). A classification similar to the one of Section (2.3) can be stated for S^I , in particular the limit cases of (62) and (63) can be envisioned, that is, (i) the *hard interface* for $\sigma_y^I \rightarrow \infty$, in which case (62) becomes $\dot{\mathbf{e}}^p = \mathbf{0}$ on S^I (dislocations cannot cross the interface), and (ii) the *free interface* for $\sigma_y^I = \psi^I = 0$, in which case (63) becomes $\langle \mathbf{q} \rangle = \mathbf{0}$ on S^I (dislocations can cross freely the interface). In intermediate situations, a part of dislocations may accumulate in the interface to promote hardening (if any). The maximum dissipation principle (31) and the minimum principle (35) can be extended straightforwardly to include the interface, but this issue is skipped for brevity.

4. Application

The shear model of Fig. 2 has been chosen for a simple application. The bulk material undergoes a displacement $u = u(y)$ in the x direction only, with consequent shear strain

$du/dy = \gamma = \tau/G + \gamma_p$, where τ is the (constant) shear stress, G the elastic shear modulus, and $\gamma_p = \gamma_p(y)$ the shear strain. The upper boundary plane ($y = H$), which undergoes a given displacement $\bar{u} = H\Gamma$, is treated as a hard surface. The lower boundary plane ($y = 0$), which is fixed, is instead treated as a boundary layer with surface tension (τ_0) and surface energy (φ). The bulk and layer hardening potentials read:

$$\psi_p = \frac{1}{2} h \left[\gamma_p^2 + \ell^2 (\gamma_p')^2 \right], \quad \varphi = \frac{1}{2} \beta \gamma_p^2, \quad (64)$$

where the prime denotes derivative with respect to y , and h, β are positive hardening moduli. From (64) we obtain the respective hardening laws as

$$X = h(\gamma_p - \ell^2 \gamma_p''), \quad Q = \beta \gamma_p. \quad (65)$$

The loading process, which is guided by a monotonically increasing (mean shear strain) Γ , by assumption does not lead to elastic unloadings, hence the deformation theory of plasticity is applied in the following analysis. For this purpose, the bulk and layer yield conditions can be written as:

$$f = \tau - X - \tau_y \leq 0, \quad \text{for } 0 < y < H, \quad (66)$$

$$f^S = q - Q - \tau_0 \leq 0, \quad \text{for } y = 0, \quad (67)$$

where τ_y and τ_0 are the respective yield stresses, whereas q denotes the applied tension given by

$$q = \ell^2 h \gamma_p''(0). \quad (68)$$

After an initial elastic regime, plastic deformation starts at $\tau = \tau_y$, or equivalently, at $\Gamma = \Gamma_e := \tau_y/G$. In the elastic–plastic regime, the yield condition (66) is satisfied as an equality and, by (65)₁, gives

$$\gamma_p - \ell^2 \gamma_p'' = \frac{\tau - \tau_y}{h}, \quad (0 < y < H). \quad (69)$$

The solution $\gamma_p(y)$ of the latter differential equation, taking into account the higher order boundary condition at the (hard) boundary $y = H$, i.e. $\gamma_p(H) = 0$, is found to be:

$$\gamma_p = \frac{\tau - \tau_y}{h} \left\{ 1 - \frac{\cosh(y/\ell)}{\cosh(H/\ell)} + C [\sinh(y/\ell) - \tanh(H/\ell) \cosh(y/\ell)] \right\}, \quad (70)$$

in which C is some constant. Analogously, using the relation $u' = \tau/G + \gamma_p$, by an integration and with the (standard) boundary conditions $u(0) = 0$ and $u(H) = H\Gamma$, we obtain:

$$\Gamma = \frac{\tau}{G} + \frac{\tau - \tau_y}{h} \frac{\ell}{H} \left[\frac{H}{\ell} - \tanh(H/\ell) - C \frac{\cosh(H/\ell) - 1}{\cosh(H/\ell)} \right]. \quad (71)$$

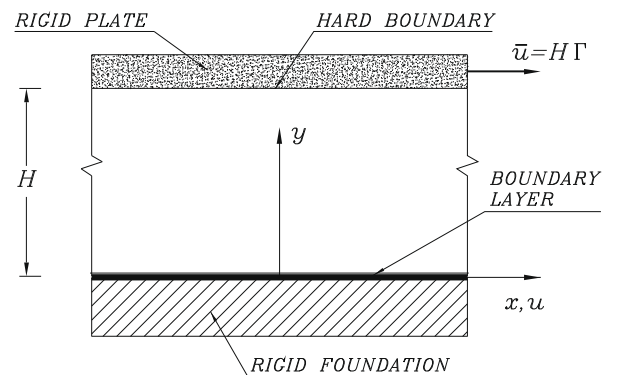


Fig. 2. Geometrical sketch of a shear model confined between a fixed stiff boundary surface on the lower side ($y = 0$) and a hard boundary surface on the upper side ($y = H$), where the imposed displacement $u(H) = H\Gamma$ increases monotonically.

4.1. First elastic–plastic regime

Just after the elastic limit is reached ($\tau = \tau_y$, $\Gamma = \Gamma_e$), the layer's yield condition is not reached yet ($f^s < 0$), hence $\gamma_p(0) = 0$, that is, the layer is not plastically active correspondingly. For shortness, let us introduce the coefficients $\xi := H/\ell$ (size ratio), $a := h/H$, $b_0 := \tau_0/(\tau_y H)$, $b_1 := \beta/(hH)$. On imposing the condition $\gamma_p(0) = 0$, the constant C is found to be given by

$$C = C_1 := \frac{\cosh \xi - 1}{\sinh \xi}. \quad (72)$$

On substituting from the latter into (70), the right plastic shear strain distribution is found for the regime being considered. An analogous substitution of C into (71) gives the relation

$$\frac{\tau}{\tau_y} = 1 + k_1(\Gamma - \Gamma_e), \quad (\Gamma \geq \Gamma_e), \quad (73)$$

where we have set:

$$k_1 := k_0/\Omega_1, \quad k_0 := G/\tau_y = \Gamma_e^{-1} \quad (74)$$

$$\Omega_1 := 1 + \frac{1}{a} \left(1 - \frac{2(\cosh \xi - 1)}{\xi \sinh \xi} \right). \quad (75)$$

The first elastic–plastic regime stops when the layer's yield condition is reached, that is, by (67) and (68) and considering that $Q = 0$ at this stage, when $h\ell^2\gamma_p'(0) = \tau_0$. The latter condition leads to the relation

$$\frac{\tau_c}{\tau_y} = 1 + b_0 \frac{\xi \sinh \xi}{\cosh \xi - 1}, \quad (76)$$

where τ_c denotes the τ value at which the first elastic–plastic regime terminates and the second one begins. Denoting by Γ_c the corresponding Γ value, we can write, by (73):

$$\Gamma_c = \Gamma_e + (\tau_c - \tau_y)/(\tau_y k_1). \quad (77)$$

The total bulk plastic dissipation power, $\mathcal{D} = \tau_y \int_0^H \gamma_p(y) dy$, is found to be:

$$\mathcal{D} = \mathcal{D}_1 := \tau_y H a [k_0 \Gamma - 1 - k_1(\Gamma - \Gamma_e)], \quad (\Gamma_e \leq \Gamma \leq \Gamma_c). \quad (78)$$

Obviously, no plastic dissipation occurs in the layer in this regime.

4.2. Second elastic–plastic regime

For $\tau > \tau_c$, or equivalently for $\Gamma > \Gamma_c$, it is $f^s = 0$, that is, by (67) and (68),

$$h\ell^2\gamma_p'(0) - \beta\gamma_p(0) = \tau_0. \quad (79)$$

This equality, implying that the boundary layer is plastically active, remembering (70) and (71), leads to

$$C = C_2 := \left(\frac{b_1(\cosh \xi - 1)}{\cosh \xi} + \frac{b_0}{(\tau - \tau_y)/\tau_y} \right) \frac{\xi}{1 + b_1 \xi \tanh \xi}, \quad (80)$$

$$\frac{\tau}{\tau_y} = \frac{\tau_c}{\tau_y} + k_2(\Gamma - \Gamma_c), \quad (\Gamma \geq \Gamma_c), \quad (81)$$

where

$$k_2 := k_0/\Omega_2, \quad (82)$$

$$\Omega_2 := \Omega_1 + \frac{1}{a} \frac{(\cosh \xi - 1)^2}{\xi \sinh \xi \cosh \xi [1 + b_1 \xi \tanh \xi]}. \quad (83)$$

Substituting C from (80) into (70) gives the right plastic shear strain distribution for the second regime. The total bulk dissipation power, \mathcal{D} , and the layer dissipation power, \mathcal{D}_0 , are easily found to be:

$$\mathcal{D} = \mathcal{D}_2 := \mathcal{D}_1 - \tau_y H a k_2 (\Gamma - \Gamma_c), \quad (\Gamma \geq \Gamma_c), \quad (84)$$

$$\mathcal{D}_0 = \tau_y H b_0 \gamma_p(0). \quad (85)$$

4.3. Graphical description of the results

The above results are diagrammatically described in the following for $k_0 = 300$ and with adimensional parameters a , b_0 , b_1 and ξ fixed at values indicated in the relevant figures.

Fig. 3 reports the quantity Γ_c as function of the size ratio ξ . It shows that $\Gamma_c - \Gamma_e$ increases monotonically with ξ , which means that $\Gamma_c \rightarrow \infty$ for $\xi \rightarrow \infty$ (macroscopic scales), $\Gamma_c \rightarrow \Gamma_e$ for $\xi \rightarrow 0$ (micro/nano scales). For every fixed Γ there exists a critical size ratio, say ξ_c , such that the corresponding plastic strain response belongs to the first elastic–plastic regime for every $\xi > \xi_c$, but to the second one for $\xi < \xi_c$.

Fig. 4a shows the γ_p profiles for $\Gamma - \Gamma_e = 0.03$ (for which $\xi_c \simeq 8$) and for different values of ξ , i.e. the values 20 and 10 (for which the boundary layer is not active) and the values 5 and 2.5 (for which the boundary layer is active). Fig. 4b provides analogous γ_p profiles for $\Gamma - \Gamma_e = 0.06$ (for which $\xi_c \simeq 17.5$) and for the same set of ξ values as in Fig. 4a, but this time the layer is inactive for $\xi = 20$, active for $\xi = 2.5, 5, 10$. These strain profiles are qualitatively in agreement with the analogous results derived by Anand et al. (2005) for a strip like the present one, but without boundary layer, as well as by Bittencourt et al. (2003) for a discrete dislocation model within crystal plasticity.

Fig. 5 reports the τ – Γ curves for different values of ξ . These plots show (energetic) size effects with decreasing ξ , as long with how the second knee of every curve (which relates to the transition from the first elastic–plastic regime to the second one) correspondingly approaches to the first knee (elastic limit). This is in perfect agreement with analogous results by Aifantis et al. (2006) relative to a bar model in extension with an interface layer in the middle section, and in part with results by Abu Al-Rub (2008) relative to a thin film confined by a boundary layer and a free plane surface.

Fig. 6 reports the plastic shear strain of the boundary layer, $\gamma_p(0)$, plotted as a function of ξ , this strain being produced under the load and structural conditions equal to those of Fig. 4b. This plot shows that the layer's plastic strain increases as ξ decreases from the relevant ξ_c value ($\simeq 17.5$ in this case), takes a peak value at a size ratio close to $\xi \simeq 1$, then falls sharply to zero for $\xi \rightarrow 0$. A similar pattern is exhibited by the layer's dissipation \mathcal{D}_0 as a function of ξ , Eq. (85). Such a behavior may perhaps be reasonably explained, for instance in terms of reduction of the bulk dislocation population for very small size ratios, say $\xi < 1$, but one has to recognize that at such scales the continuum model likely fails to hold and that an atomistic view point would be more appropriate.

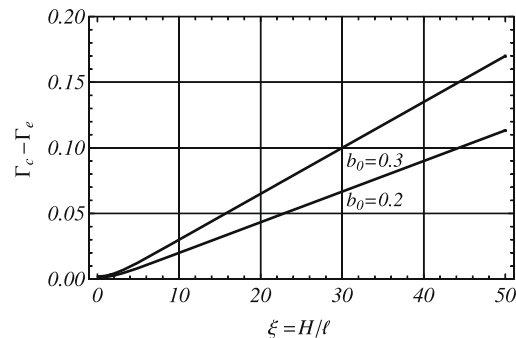


Fig. 3. Imposed mean shear strain value, Γ_c , on the shear model of Fig. 2, at which the first elastic–plastic regime terminates and the second one begins, plotted as a function of the size ratio $\xi = H/\ell$, for two values of the adimensional surface tension, b_0 , and for $a = h/G = 0.4$, $b_1 = \beta/(hH) = 0.75$.

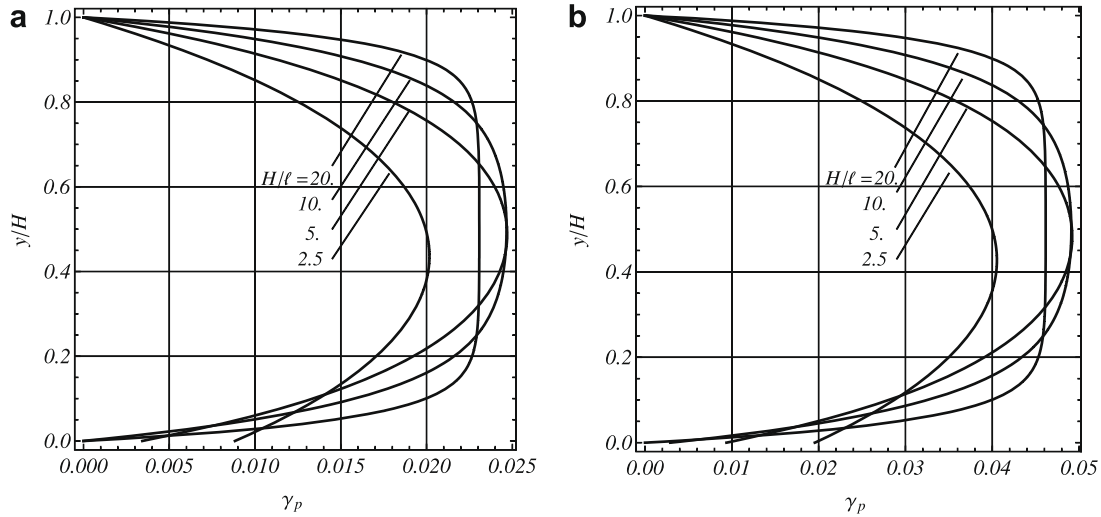


Fig. 4. Plastic shear strain profiles relative to the shear model of Fig. 2 with different values of the size ratio $\xi = H/\ell$ and for $a = h/G = 0.4$, $b_0 = \tau_0/(\tau_y) = 0.3$, $b_1 = \beta/(hH) = 0.75$, under an imposed mean plastic shear strain $\Gamma - \Gamma_e = 0.03$ (a) and $\Gamma - \Gamma_e = 0.06$ (b).

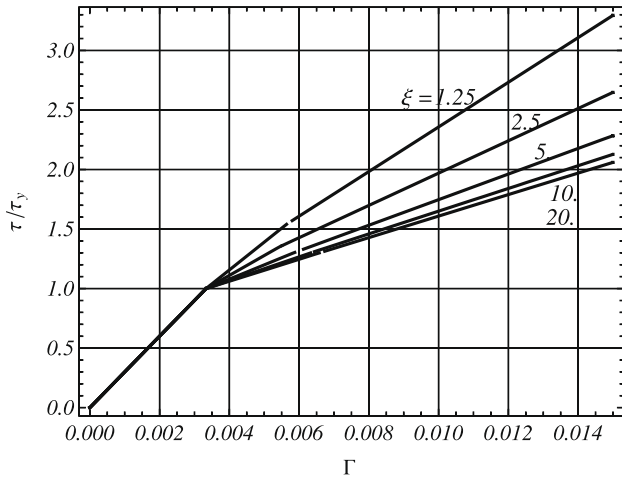


Fig. 5. $\tau - \Gamma$ diagrams relative to the shear model of Fig. 2, for different values of the size ratio $\xi = H/\ell$ and for $a = h/G = 0.4$, $b_0 = \tau_0/(\tau_y H)$, $b_1 = \beta/(hH) = 0.75$.

5. Conclusion

Interfacial energy effects – which manifest themselves in the framework of gradient plasticity whenever the solid includes boundary layers, i.e. boundary surfaces and/or interfaces each featured by a surface tension and a surface energy – have been addressed making use of the residual-based strain gradient plasticity theory. It has been shown that the latter theory – provided the *insulation condition*, on which it grounds, comprises both the bulk material and the layer(s) – constitutes a suitable means to derive, in a form consistent with thermodynamics principles, all the state equations, as well as the right expressions of the dissipation power density and the residual, for both the bulk material and the layer(s).

Coupled evolution laws of rate independent associative plasticity have been provided for the bulk material and for the layer(s). Whereas the bulk material obeys a kinematically hardening law in the form of PDEs with related higher order boundary conditions, the boundary layer obeys a finite (i.e. nondifferential) hardening law. A coupled maximum dissipation principle has been shown to hold. The problem of determining the stress and plastic strain state for a body being in a given total strain and subjected to a

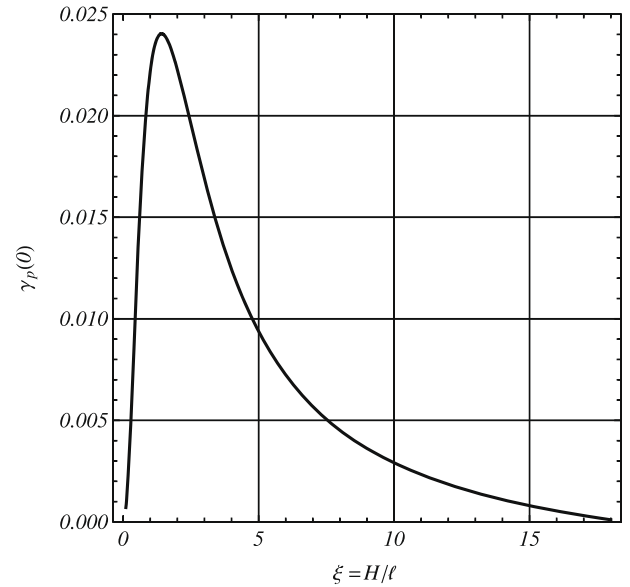


Fig. 6. Plastic shear strain in the boundary layer for the load and structural conditions of Fig. 4b, plotted as a function of the size ratio $\xi = H/\ell$.

specified plastic strain rate field, has been found to be governed by a minimum principle, equivalent to a PDE problem.

The higher order boundary conditions have been studied in details and categorized in relation to some peculiar features of the boundary surface. Four categories of such boundary surfaces have been recognized, i.e. (i) *hard boundary surface*: infinite surface tension; zero plastic strain; (ii) *stiff boundary surface*: finite surface tension; equal plastic strain in the boundary surface and the adjacent bulk material (this case includes the previous one as a limit case); (iii) *soft boundary surface*: zero surface tension, but nonzero surface energy; applied tension equal to the layer's hardening force; (iv) *free boundary surface*: zero surface tension and surface energy; zero applied tension (this case in a limit situation of the previous one). The higher order boundary conditions have been recognized to possess a basic role in the coupling of the plasticity flow laws of the boundary layer and the adjacent bulk material.

The results provided in the present paper substantially conform to concepts and notions known in the literature (herein quoted),

but some improvements have been also given. These include: a categorization of the higher order boundary conditions, the coupling of the bulk/layer evolution laws and its relationship with the higher order boundary conditions, a global maximum dissipation principle for the aforementioned laws, a minimum principle for the evaluation of the stress and plastic strain states in a body being in a given total strain state and subjected to a specified plastic strain rate field.

References

- Abu Al-Rub, R.K., 2008. Interfacial gradient plasticity governs scale-dependent yield strength and strain hardening rates in micro/nano structural metals. *Int. J. Plasticity* 24, 1277–1306.
- Abu Al-Rub, R.K., Voyiadjis, G.Z., Bommann, D.J., 2007. A thermodynamics based higher-order gradient theory for size dependent plasticity. *Int. J. Solids Struct.* 44, 2888–2923.
- Aifantis, K.E., Willis, J.R., 2005. The role of interfaces in enhancing the yield strength of composites and polycrystals. *J. Mech. Phys. Solids* 53, 1047–1070.
- Aifantis, K.E., Willis, J.R., 2006. Scale effects induced by strain-gradient plasticity and interfacial resistance in periodic and randomly heterogeneous media. *Mech. Mater.* 38, 702–716.
- Aifantis, K.E., Soer, W.A., De Hosson, J.Th.M., Willis, J.R., 2006. Interfaces within strain gradient plasticity: theory and experiments. *Acta Mater.* 54, 5077–5085.
- Anand, L., Gurtin, M.E., Lele, S.P., Gething, C., 2005. A one-dimensional theory of strain-gradient plasticity: Formulation, analysis, numerical results. *J. Mech. Phys. Solids* 53, 1789–1826.
- Ashby, M.F., 1970. The deformation of plastically non-homogeneous materials. *Philos. Mag.* 21, 399–424.
- Bardella, L., 2008. A comparison between crystal and isotropic strain gradient plasticity theories with accent on the role of the plastic spin. *Eur. J. Mech. A/Solids*. doi:10.1016/j.euromechsol.2008.10.006.
- Bittencourt, E., Needleman, A., Gurtin, M.E., Van der Gissen, E., 2003. A comparison of nonlocal continuum and discrete dislocation of plasticity predictions. *J. Mech. Phys. Solids* 51, 281–310.
- Borg, U., Fleck, N.A., 2007. Strain gradient effects in surface roughening. *Modelling Simul. Mater. Sci. Eng.* 15, 1–12.
- Borino, G., Polizzotto, C., 2007. A thermodynamically consistent gradient plasticity theory and comparison with other formulations. *Model. Mater. Sci. Eng.* 15, 23–35.
- Cermelli, P., Gurtin, M.E., 2002. Geometrically necessary dislocations in viscoplastic single crystals and bicrystals undergoing small deformations. *Int. J. Solids Struct.* 39, 6281–6309.
- Colemann, B.D., Gurtin, M.E., 1967. Thermodynamics with internal variables. *J. Chem. Phys.* 47, 597–613.
- Fleck, N.A., Hutchinson, J.W., 2001. A reformulation of strain gradient plasticity. *J. Mech. Phys. Solids* 49, 2245–2271.
- Fleck, N.A., Willis, J.R., 2008. A mathematical basis for strain-gradient plasticity theory – Part I: scalar plastic multiplier. *J. Mech. Phys. Solids*. doi:10.1016/j.jmps.2008.09.010.
- Fredriksson, P., Gudmundson, P., 2005. Size-dependent yield strength of thin films. *Int. J. Plasticity* 21, 1834–1854.
- Fredriksson, P., Gudmundson, P., 2007a. Modelling of interface between a thin film and a substrate within a strain gradient plasticity framework. *J. Mech. Phys. Solids* 55, 939–955.
- Fredriksson, P., Gudmundson, P., 2007b. Competition between interface and bulk dominated plastic deformation in strain gradient plasticity. *Model. Simul. Mater. Sci. Eng.* 15, 61–69.
- Germain, P., Nguyen, Q.S., Suquet, P., 1983. Continuum thermodynamics. *ASME J. Appl. Mech.* 50, 1010–1021.
- Gudmundson, P., 2004. A unified treatment of strain gradient plasticity. *J. Mech. Phys. Solids* 52, 1377–1406.
- Gurtin, M.E., 2004. A gradient theory of small-deformation isotropic plasticity that accounts for the Burgers vector and for dissipation due to plastic spin. *J. Mech. Phys. Solids* 52, 2545–2568.
- Gurtin, M.E., Anand, L., 2005. A theory of strain-gradient plasticity for isotropic, plastically irrotational materials. Part I: small deformation. *J. Mech. Phys. Solids* 53, 1624–1649.
- Gurtin, M.E., Needleman, A., 2005. Boundary conditions in small-deformation, single-crystal plasticity that account for the Burgers vector. *J. Mech. Phys. Solids* 53, 1–31.
- Lemaitre, J., Chaboche, J.-L., 1990. *Mechanics of Solid Materials*. Cambridge University Press, Cambridge.
- Menzel, A., Steinmann, P., 2000. On the continuum formulation of higher gradient plasticity for single and polycrystals. *J. Mech. Phys. Solids* 48, 1777–1796.
- Polizzotto, C., 2003. Unified thermodynamic framework for nonlocal/gradient continuum theories. *Eur. J. Mech. A/Solids* 22, 651–668.
- Polizzotto, C., 2007. Strain-gradient elastic–plastic material models and assessment of the higher order boundary conditions. *Eur. J. Mech. A/Solids* 26, 189–211.
- Polizzotto, C., 2008. Thermodynamics-based gradient plasticity theories with an application to interface models. *Int. J. Solids Struct.* 45, 4820–4834.
- Polizzotto, C., Borino, G., 1998. A thermodynamics-based formulation of gradient dependent plasticity. *Eur. J. Mech. A/Solids* 17, 741–761.
- Polizzotto, C., Fuschi, P., Pisano, A.A., 2006. A nonhomogeneous nonlocal elasticity model. *Eur. J. Mech. A/Solids* 25, 308–333.
- Svedberg, T., Runesson, K., 1998. An algorithm for regularized plasticity coupled to damage based on dual mixed FE-formulation. *Comput. Meth. Appl. Mech. Eng.* 161, 49–65.